

Fig. 1

Residual Form Method to compute ρ_q and ρ_u	Direct Form Method to compute \dot{q} and \dot{u}
<ol style="list-style-type: none"> 1. Compute the First Kinematics Calc. and the kinematic residual $\rho_q(k)$ 2. Generate $\hat{T}(k)$, the spatial load balance for each body 3. Compute dynamic residual $\rho_u(k)$ 	<ol style="list-style-type: none"> 1. Compute \dot{q} using joint specific routines 2. Perform First Kinematics Calc. with $\dot{u}=0$ 3. Generate residuals ρ_u and negate $\rho_u = -\rho_u$ 4. Perform Second Kinematics Calc. 5. Compute \dot{u} using Forward Dynamics

Comparison of Methods
Fig. 5



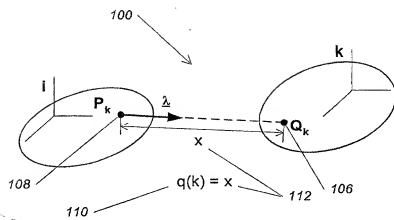


Fig. 4A

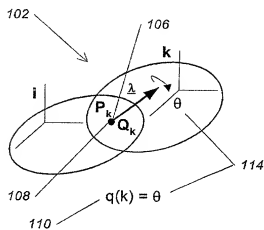


Fig. 4B

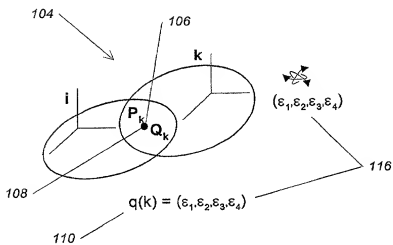


Fig. 4C

Molecule	No. Residues in polypeptide	No. Atoms	Direct Form Approximate Operation Count	Residual Form Approximate Operation Count	Factor of Speed Up
Alanine Dipeptide	2	23	4,991	683	7.31
20-mer Polyalanine	20	257	42,340	5,894	7.24
100-mer Polyalanine	100	1297	207,018	28,973	7.15

Computation Comparison

Fig. 6